

RNN with Particle Flow for Probabilistic Spatio-temporal Forecasting

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Introduction

- Exploit underlying graph structure for time series forecasting

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- Applications: road traffic, wireless networks

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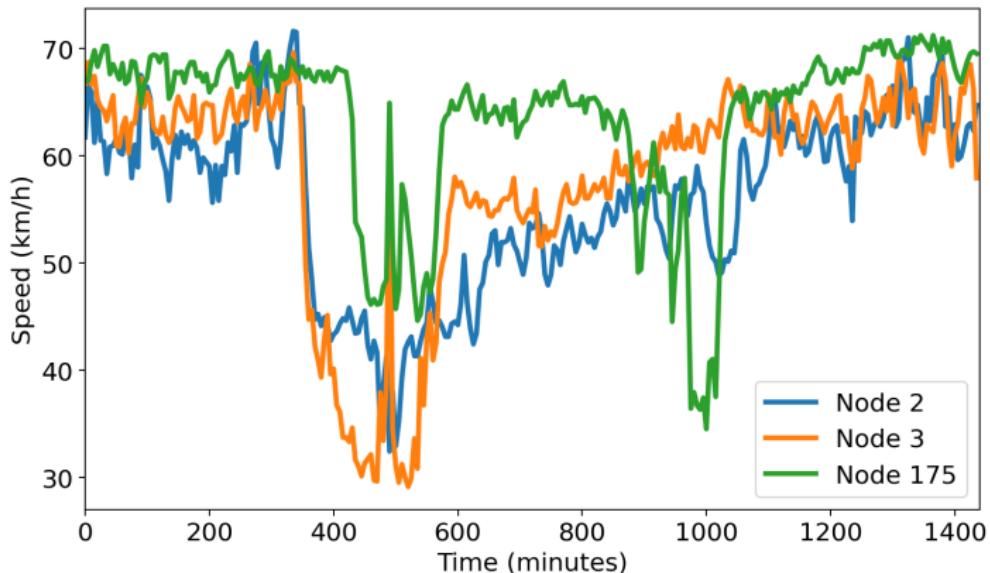


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- *State-of-the-art*
 - Graph convolution + recurrent networks¹
 - Temporal convolution²
 - Attention mechanism³

¹ Li et al. 2018, Bai et al. 2020

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- Provide point forecast, **no measure of uncertainty**
- Existing probabilistic models⁴ **cannot process a graph.**
- This work: Bayesian framework to assess forecast uncertainty

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Problem Formulation

State-space model

Initial state distribution: $x_1 \sim p_1(\cdot, z_1, \rho)$,

State transition model: $x_t = g_{\mathcal{G}, \psi}(x_{t-1}, y_{t-1}, z_t, v_t)$, for $t > 1$,

Emission model: $y_t = h_{\mathcal{G}, \phi}(x_t, z_t, w_t)$, for $t \geq 1$.

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- $g_{\mathcal{G}, \psi}$: GNN+RNN (e.g. AGCRU⁵, DCGRU⁶)

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- $h_{\mathcal{G}, \phi}$: NN (e.g. linear layer)
- Unknown model parameters: $\Theta = \{\rho, \psi, \sigma, \phi, \gamma\}$

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Diffusion Convolutional GRU

$$r_t = \sigma(W_r \star_{\mathcal{G}} [y_t, x_{t-1}] + b_r)$$

$$u_t = \sigma(W_u \star_{\mathcal{G}} [y_t, x_{t-1}] + b_u)$$

$$c_t = \tanh(W_c \star_{\mathcal{G}} [y_t, (r_t \odot x_{t-1})] + b_c)$$

$$x_t = u_t \odot x_{t-1} + (1 - u_t) \odot c_t$$

An Example of $g_{\mathcal{G}, \psi}$

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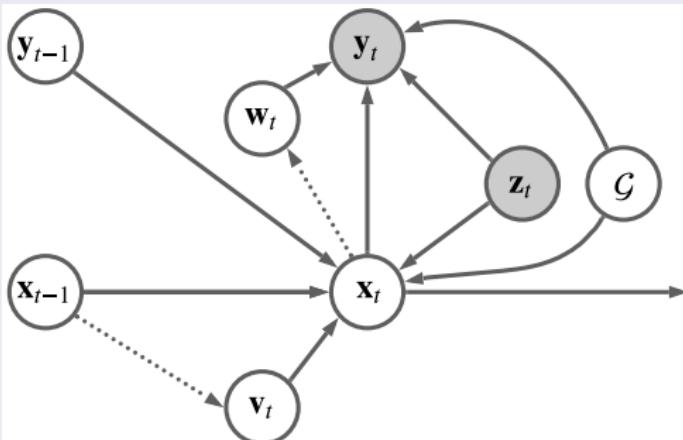
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$T_k(\cdot)$: k -th order Chebyshev polynomial

D_O, D_I : out-degree, in-degree matrices, A : adjacency

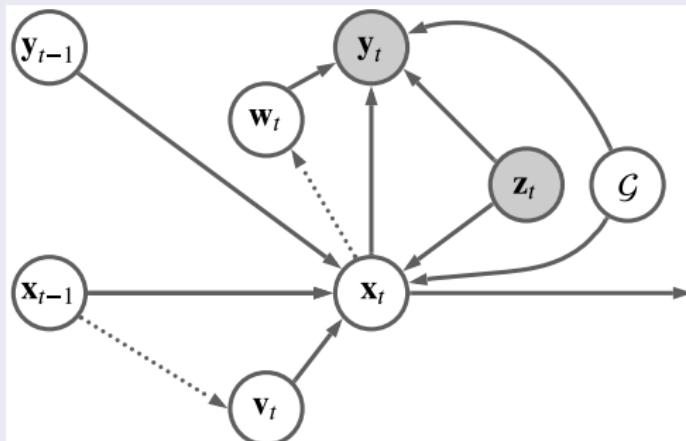
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Graphical model representation



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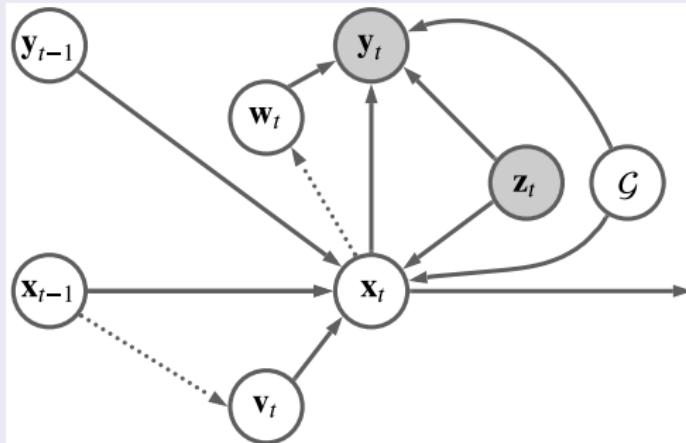


Task

Predict $y_{t_0+P+1:t_0+P+Q}$ based on $y_{t_0+1:t_0+P}$, $z_{t_0+1:t_0+P+Q}$, and (possibly) \mathcal{G}

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Graphical model representation



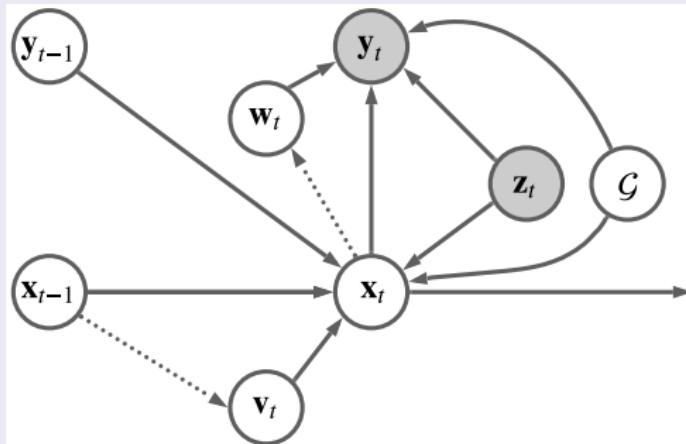
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- Train the model to learn Θ
- Approximate $p_\Theta(y_{P+1:P+Q}|y_{1:P}, z_{1:P+Q})$ for test data

Computing Forecast Distribution

$$p_{\Theta}(y_{P+1:P+Q} | y_{1:P}, z_{1:P+Q}) = \int \prod_{t=P+1}^{P+Q} \left(p_{\phi,\gamma}(y_t | x_t, z_t) \right. \\ \left. p_{\psi,\sigma}(x_t | x_{t-1}, y_{t-1}, z_t) \right) \\ p_{\Theta}(x_P | y_{1:P}, z_{1:P}) dx_{P:P+Q} .$$

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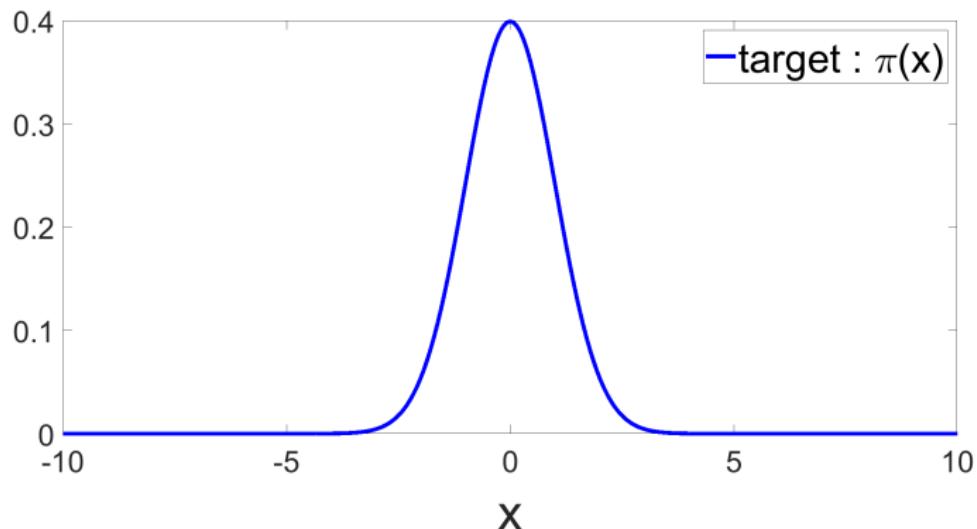
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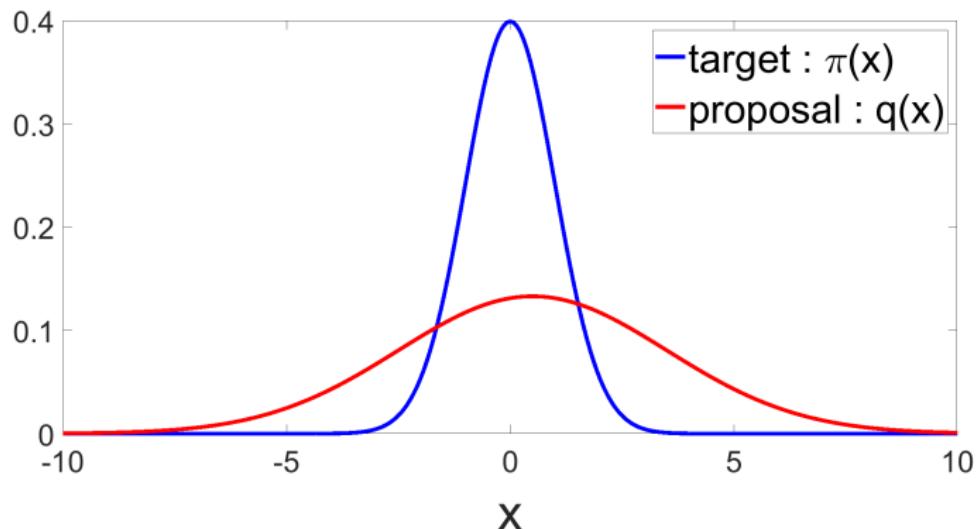
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- $p_{\phi,\gamma}(y_t|x_t, z_t)$: sampling forecast using $h_{\mathcal{G},\phi}$

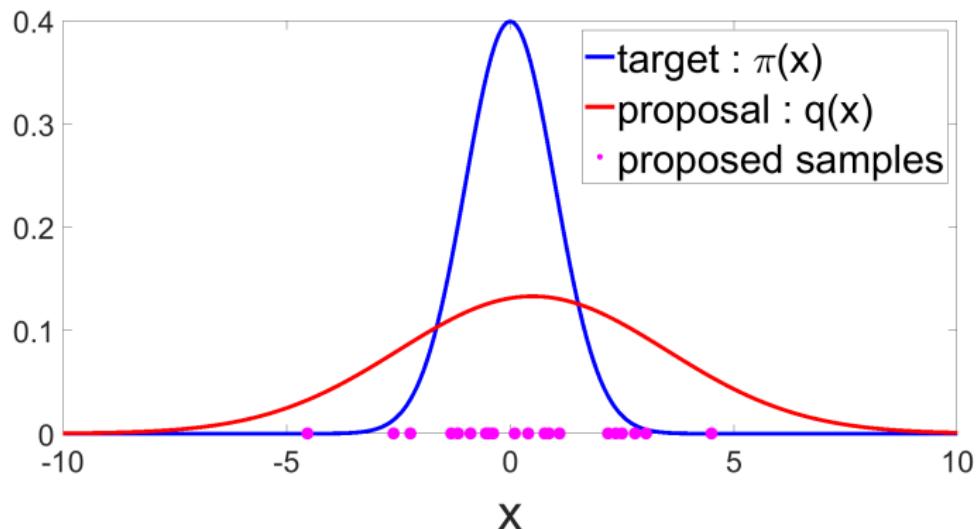
Importance Sampling



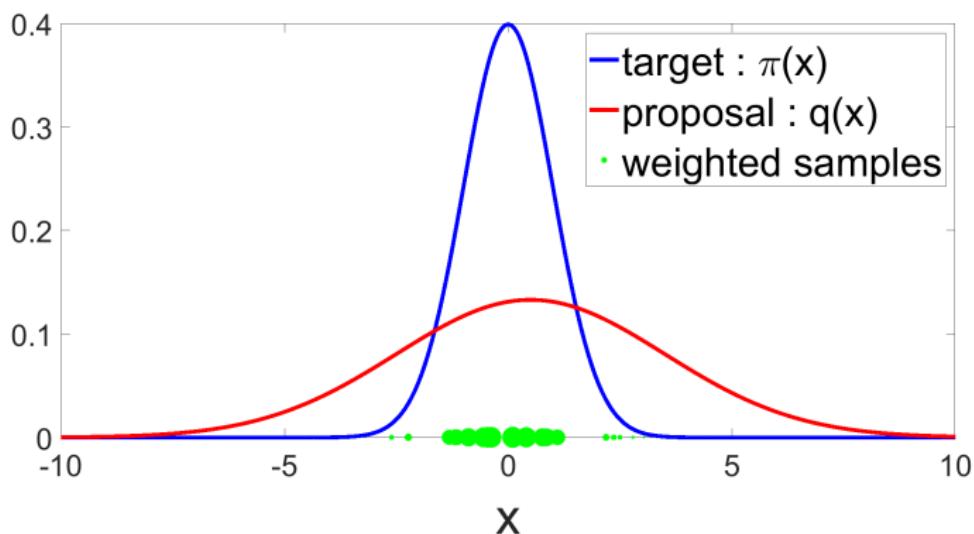
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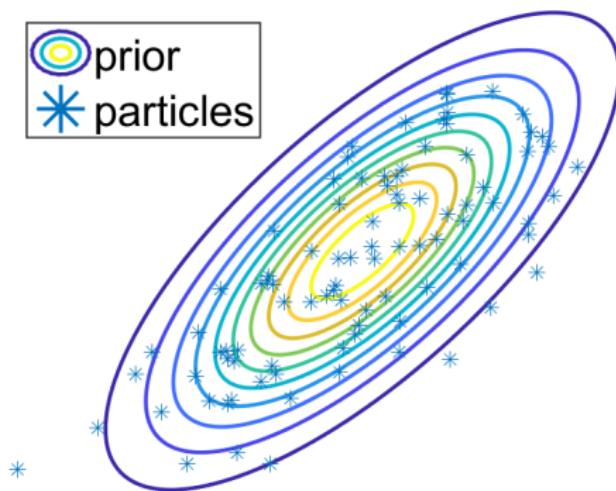


Particle Filter: Weight Degeneracy

Particle filter suffers from **weight degeneracy** for **high dimensional state/ informative observations.**

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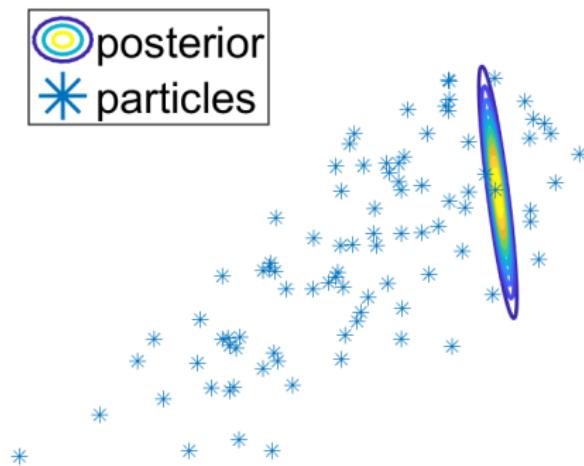
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Contours of the prior distribution

Particle Filter: Weight Degeneracy

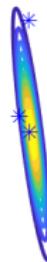
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Contours of the posterior distribution

Particle Filter: Weight Degeneracy

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Resampling of the particles

Particle Flow

Particles flow⁷ **migrates** particles from the prior to the posterior distribution.

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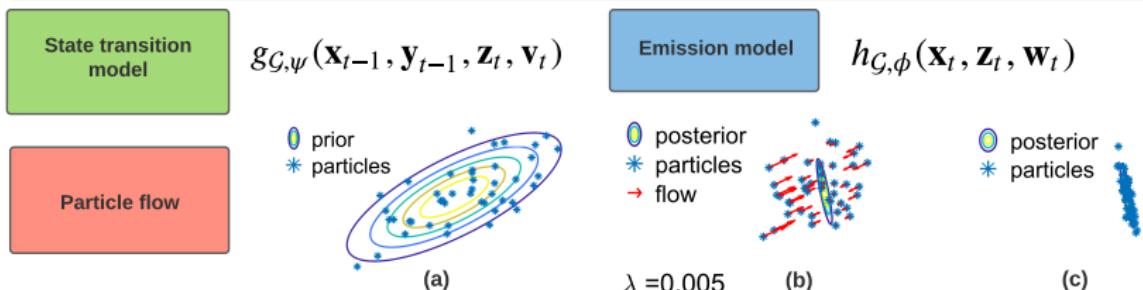
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(a) Samples (asterisk) from the prior distribution

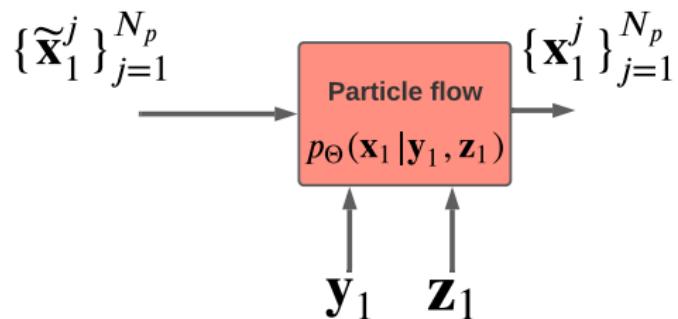
(b) Contours of the posterior distribution and the direction of flow for the particles at an intermediate step

(c) Particles after the flow, approximately distributed according to the posterior distribution

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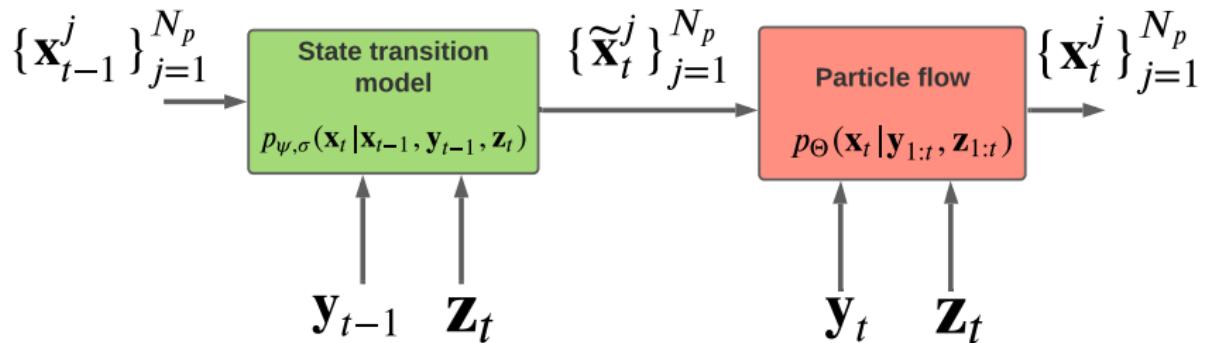
$$t = 1$$

$$\{\tilde{\mathbf{x}}_1^j\}_{j=1}^{N_p} \sim p_1(\cdot, \mathbf{z}_1, \rho)$$



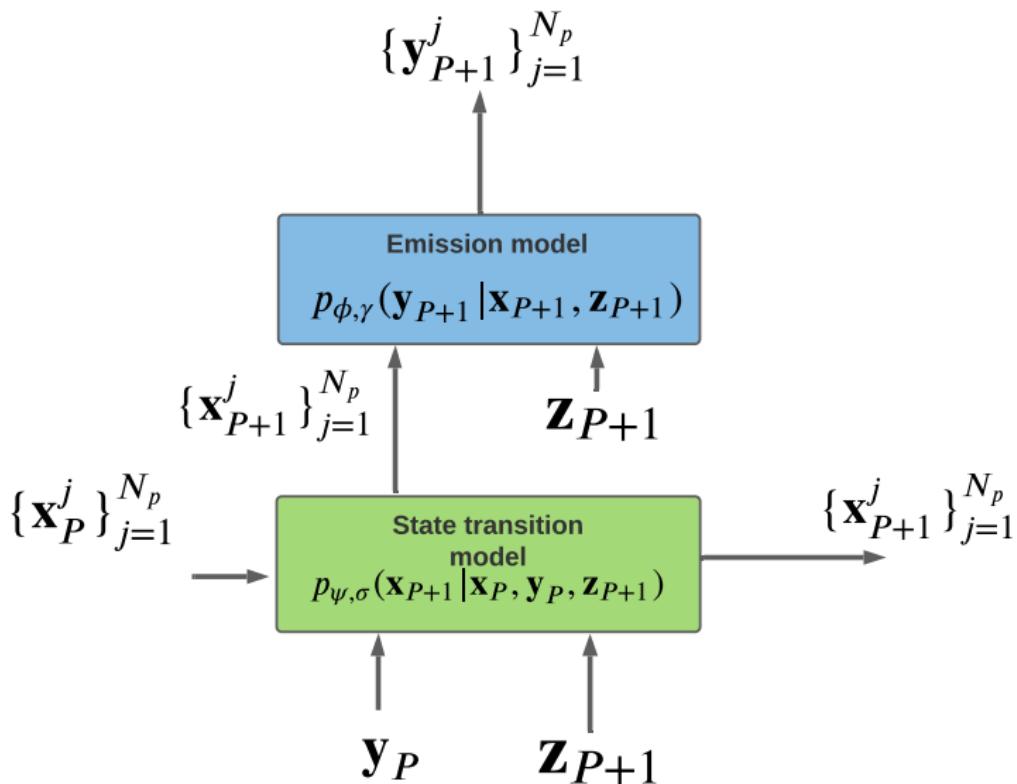
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$$2 \leq t \leq P$$



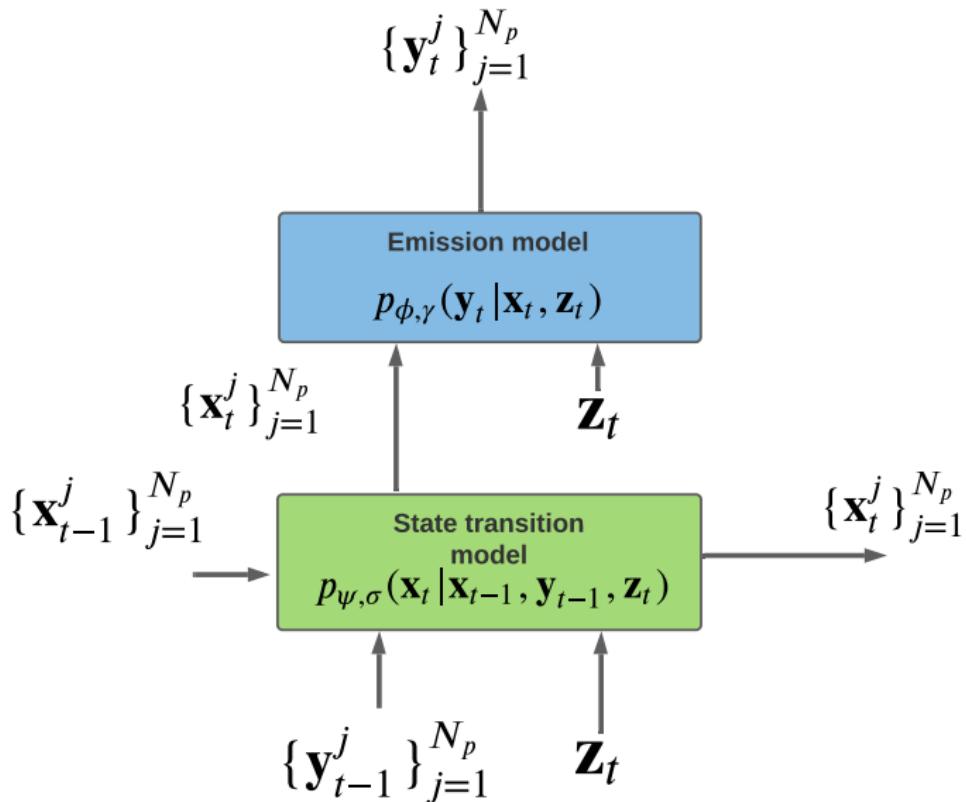
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$$t = P + 1$$

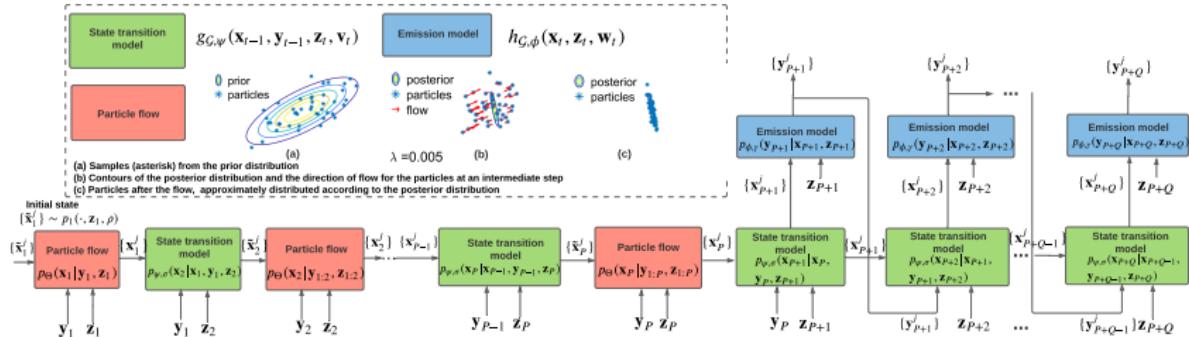


Computing Forecast Distribution

$$P + 2 \leq t \leq P + Q$$



Computing Forecast Distribution



Loss Function

- For point forecasting: MAE, MSE
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$$\mathcal{L}_{\text{prob}}(\Theta, \mathcal{D}) = -\frac{1}{|\mathcal{D}|} \sum_{n \in \mathcal{D}} \log p_{\Theta}(y_{P+1:P+Q}^{(n)} | y_{1:P}^{(n)}, z_{1:P+Q}^{(n)}),$$

$$\hat{p}_{\Theta}(y_{P+1:P+Q} | y_{1:P}, z_{P+1:P+Q}) = \prod_{t=P+1}^{P+Q} \left[\frac{1}{N_p} \sum_{j=1}^{N_p} p_{\phi,\gamma}(y_t | x_t^j, z_t) \right].$$

Experiments

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- Performance metrics for point forecasting:
 - MAE, RMSE, and MAPE
- Performance metrics for probabilistic forecasting:
 - Continuous Ranked Probability Score (CRPS)⁹
 - P10, P50, and P90 Quantile Losses¹⁰

⁸ Chen et al. 2000

⁹ Gneiting & Raftery 2007

¹⁰ Wang et al. 2019

Baselines

- Statistical and ML point forecast models:
 - HA, ARIMA¹¹, VAR¹², SVR¹³, FNN, FC-LSTM¹⁴

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- Graph agnostic probabilistic forecast models:
 - DeepAR²⁵, DeepFactors²⁶, MQRNN²⁷

¹¹ Makridakis & Hibon 1997, ¹² Hamilton 1994, ¹³ Chun-Hsin et al. 2004, ¹⁴ Sutskever et al. 2014

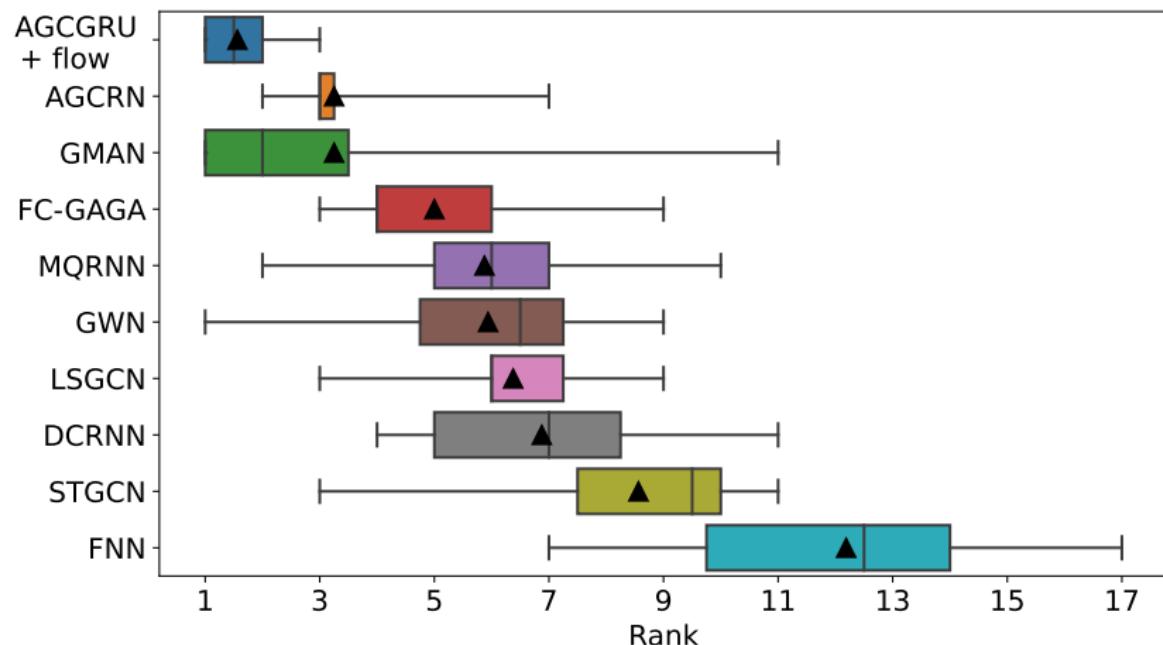
¹⁵ Li et al. 2018, ¹⁶ Yu et al. 2018, ¹⁷ Guo et al. 2019, ¹⁸ Wu et al. 2019, ¹⁹ Zheng et al. 2020,

²⁰ Bai et al. 2020, ²¹ Huang et al. 2021

²² Sen et al. 2019, ²³ Oreshkin et al. 2020, ²⁴ Oreshkin et al. 2021

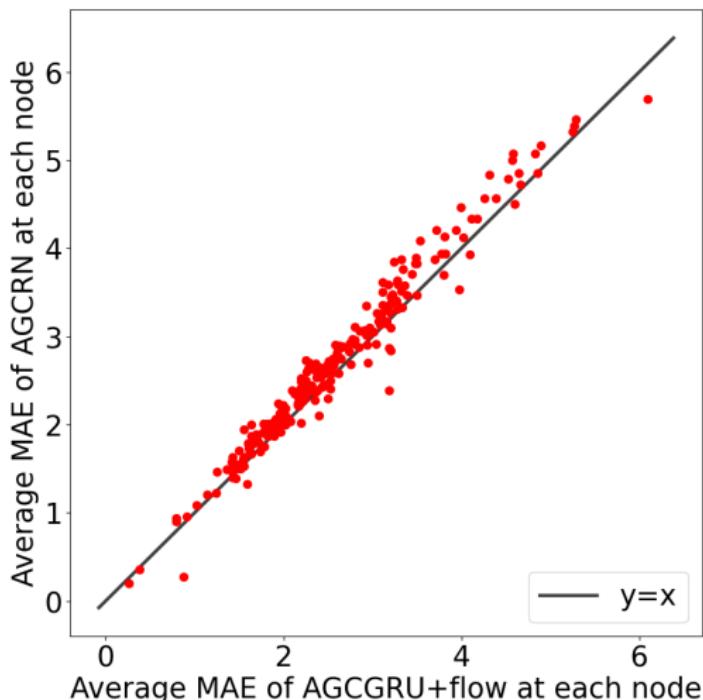
²⁵ Salinas et al. 2020, ²⁶ Wang et al. 2019, ²⁷ Wen et al. 2017

Experimental Results: Point Forecasting



AGCGRU+flow achieves the best average rank.

Experimental Results: Node by Node Comparison



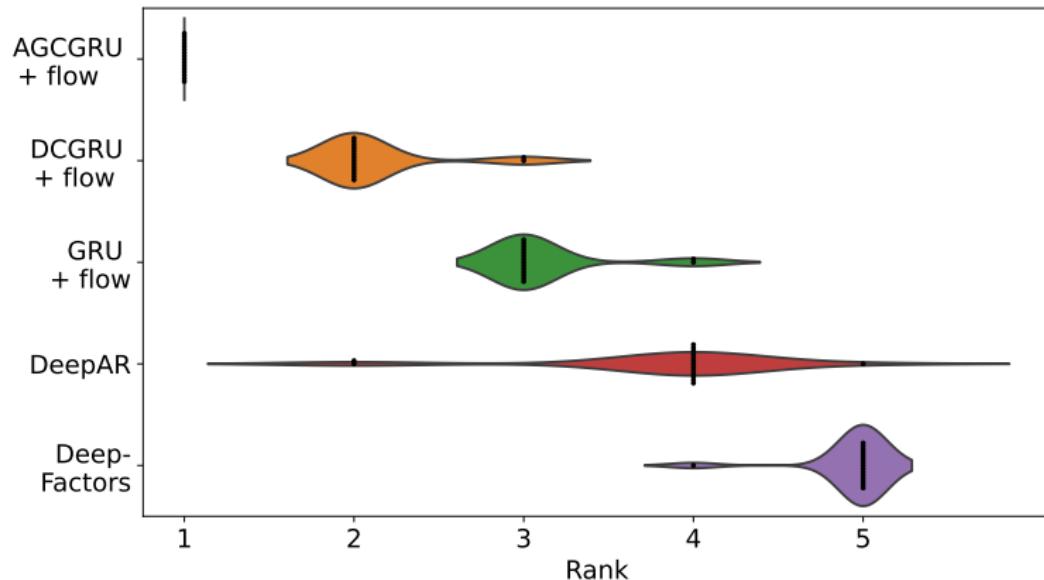
AGCGRU+flow outperforms AGCRN at majority of nodes in PeMSD7

Experimental Results: Probabilistic Forecasting

$$\text{CRPS}(F, x) = \int_{-\infty}^{\infty} \left(F(z) - 1\{x \leq z\} \right)^2 dz$$

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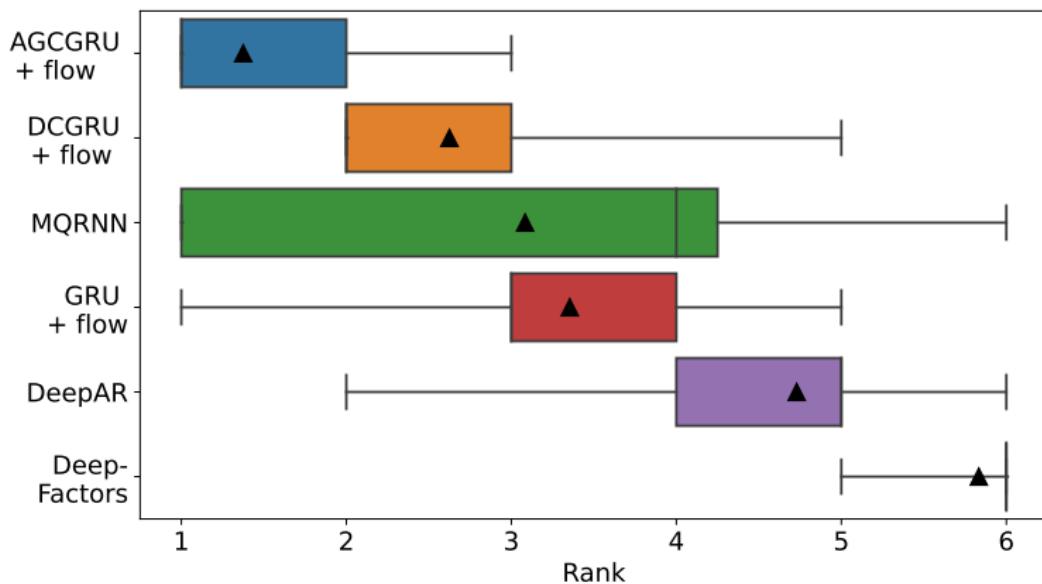
Our approaches obtain lower average CRPS.

Experimental Results: Quantile Estimation

$$QL(x, \hat{x}(\alpha)) = 2 \left(\alpha(x - \hat{x}(\alpha)) \mathbf{1}\{x > \hat{x}(\alpha)\} + (1 - \alpha)(\hat{x}(\alpha) - x) \mathbf{1}\{x \leq \hat{x}(\alpha)\} \right)$$

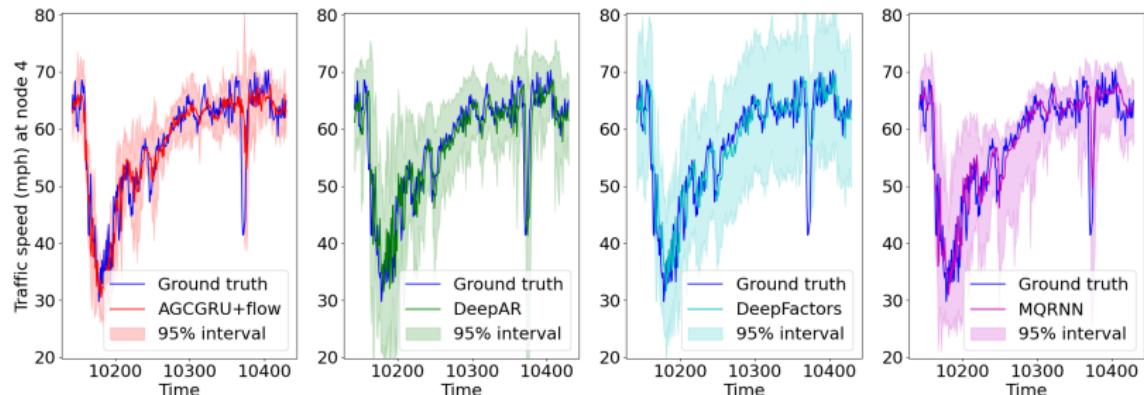
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AGCGRU+flow has the lowest quantile error on average.

Experimental Results: Confidence Intervals



Confidence intervals for 15 minutes ahead predictions at node 4 of PeMSD7 for the first day in the test set.

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- Code: https://github.com/networkslab/rnn_flow